Landau functions for non-interacting bosons

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We discuss the statistics of Bose-Einstein condensation (BEC) in a canonical ensemble of N non-interacting bosons in terms of a Landau function $\mathcal{L}_N^{\mathrm{BEC}}(q)$ defined by the logarithm of the probability distribution of the order parameter q for BEC. We also discuss the corresponding Landau function for spontaneous symmetry breaking (SSB), which for finite N should be distinguished from $\mathcal{L}_N^{\mathrm{BEC}}(q)$. Only for $N \to \infty$ BEC and SSB can be described by the same Landau function which depends on the dimensionality and on the form of the external potential in a surprisingly complex manner. For bosons confined by a three-dimensional harmonic trap the Landau function exhibits the usual behavior expected for continuous phase transitions.

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The concept of a Landau function $\mathcal{L}(p)$ has been extremely useful to understand the nature of phase transitions [1]. For example, in the vicinity of a second order (continuous) thermal phase transition $\mathcal{L}(p)$ smoothly develops minima at non-zero values of the relevant order parameter p when the temperature T drops below the critical temperature T_c, see Fig. 1 (a). On the other hand, in the case of a first order phase transition the location of the minima of $\mathcal{L}(p)$ changes discontinuously at $T = T_c$, as shown in Fig. 1(b). While for infinite systems and in the absence of spontaneous symmetry breaking (SSB) $\mathcal{L}(p)$ can be identified with the Gibbs potential, this identification is in general not valid for finite systems or in the symmetry broken phase. In the latter case the Gibbs potential, which by construction is a convex function of p, exhibits a plateau as shown in Fig. 1. Microscopically, $\mathcal{L}(p)$ is defined in terms of the logarithm of the probability distribution of the order parameter in a given statistical ensemble [1]. From this probabilistic definition it is clear that $\mathcal{L}(p)$ does not have a strictly thermodynamic interpretation.

For non-interacting systems the Landau function is in

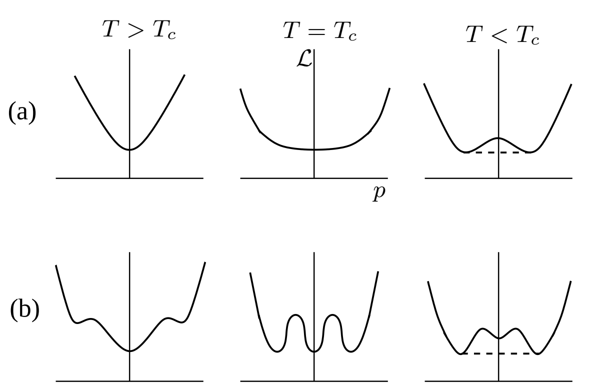

FIG. 1: Typical evolution of the Landau function $\mathcal{L}$ as a function of the relevant order parameter p close to (a) second order and (b) first order phase transitions. The dashed line denotes the plateau of the corresponding Gibbs potential for $T < T_c$.

most cases not very interesting, because the correlations responsible for phase transitions are usually due to interactions between the microscopic degrees of freedom. An important exception are non-interacting bosons, where at low temperatures the correlations imposed by quantum statistics are sufficient to give rise to a phase transition, the Bose-Einstein condensation (BEC) [2, 3]. In the condensed state the fraction of particles that occupy the single-particle state with the lowest energy is of the order of unity. More precisely, the order parameter for BEC can be chosen to be the expectation value of the operator $\hat{q} = b_0^\dagger b_0/N$, where b_0 annihilates a boson in the single-particle ground state and N is the total number of particles in the system.

Conceptually, BEC should be distinguished from SSB, which manifests itself via a finite expectation value of the operator $\hat{\phi} = b_0/\sqrt{N}$ in the limit $N \to \infty$. Of course, for any finite N there is no off-diagonal long-range order, so that $\langle \hat{\phi} \rangle = 0$. For interacting bosons in the limit $N \to \infty$ it can be shown that $\langle \hat{q} \rangle = |\langle \hat{\phi} \rangle|^2$ whenever the Bogoliubov approximation of replacing the operator b_0 by a complex number yields the right pressure [4]. For finite systems, however, one should distinguish between SSB and BEC. More precisely, both phenomena should be characterized by different probability distributions, $P_N^{\mathrm{SSB}}(\phi)$ and $P_N^{\mathrm{BEC}}(q)$, which depend on the eigenvalues q and ϕ of the operators $\hat{q}$ and $\hat{\phi}$ defined above. We parameterize the probability distributions in terms of Landau functions $\mathcal{L}_N^{\mathrm{SSB}}(\phi)$ and $\mathcal{L}_N^{\mathrm{BEC}}(q)$, see Eqs. (7,8) below. For *interacting* bosons the condensation transition is known to be second order [2], so that the Landau functions resemble in this case Fig. 1 (a). But how do the Landau functions of *non-interacting* bosons look like? Because the order parameter is continuous, the first order scenario in Fig. 1 (b) can be ruled out. In spite of the enormous activity in the field of BEC in recent years, this question has apparently not been addressed in the literature. Although the probability distribution $P_N^{\mathrm{BEC}}(q)$ has been studied by several authors [5, 6, 7, 8, 9, 10], the associated Landau function $\mathcal{L}_N^{\mathrm{BEC}}(q)$ has not been con-

sidered. The corresponding quantities for SSB have not even been properly defined in the literature.

To describe BEC experiments in finite clusters of bosonic atoms [11], we use a statistical ensemble with constant particle number N, i.e., the canonical ensemble. The mathematically more convenient grand canonical ensemble is neither relevant for experiments [11], nor is it appropriate to describe the condensed phase [7, 12]. To derive explicit expressions for $\mathcal{L}_N^{\rm SSB}(\phi)$ and $\mathcal{L}_N^{\rm BEC}(q)$, consider the canonical partition function, $Z_N = {\rm Tr}_N \exp[-\beta \hat{H}]$, where $\beta = 1/T$ is the inverse temperature and ${\rm Tr}_N$ denotes the trace over the N-particle Hilbert space of a system of non-interacting bosons with Hamiltonian $\hat{H} = \sum_{\boldsymbol{m}} E_{\boldsymbol{m}} b_{\boldsymbol{m}}^\dagger b_{\boldsymbol{m}}$. Here, $b_{\boldsymbol{m}}$ annihilates a boson in a single particle state with quantum numbers $\boldsymbol{m}$ and energy $E_{\boldsymbol{m}}$. For free bosons (FB) with mass M confined to a D-dimensional volume L^D with periodic boundary conditions $E_{\boldsymbol{m}} = (2\pi\hbar \boldsymbol{m}/L)^2/2M$, where $\boldsymbol{m}$ is a D-dimensional vector with integer components $m_i = 0, \pm1, \pm2, \ldots$, $i = 1, \ldots, D$. For bosons confined by a harmonic potential (HB) with oscillation frequency ω the energy is $E_{\boldsymbol{m}} = \hbar\omega \sum_{i=1}^{D}(m_i + 1/2)$, where $m_i = 0, 1, 2, \ldots$. For later convenience we introduce dimensionless energies $\epsilon_{\boldsymbol{m}} = \beta E_{\boldsymbol{m}}$ and the relevant dimensionless density $\rho = (\lambda_{\rm th}/L)^D N$, where for FB the thermal de Broglie wavelength is $\lambda_{\rm th} = \hbar\sqrt{2\pi\beta/M}$, whereas for HB we define $\lambda_{\rm th} = \hbar\omega\beta L$ and $L = (M\omega/\hbar)^{1/2}$.

With the help of the projection operator $\delta_{N,\hat{N}} = \int_0^{2\pi} \frac{dy}{2\pi} e^{iy(N-\hat{N})}$, where $\hat{N} = \sum_{\boldsymbol{m}} b_{\boldsymbol{m}}^\dagger b_{\boldsymbol{m}}$, we can express Z_N in terms of a trace over the entire Fock space [13],

$$Z_N = {\rm Tr}\left[\delta_{N,\hat{N}} e^{-\beta\hat{H}}\right] = \int_0^{2\pi} \frac{dy}{2\pi} e^{iyN} {\rm Tr} e^{-\beta\hat{H} - iy\hat{N}} \; . \quad (1)$$

The partial trace over the $\boldsymbol{m} \neq 0$ sector of the Fock space yields

$${\rm Tr}_{\boldsymbol{m}\neq 0} e^{-\sum_{\boldsymbol{m}\neq 0}(\epsilon_{\boldsymbol{m}} + iy) b_{\boldsymbol{m}}^\dagger b_{\boldsymbol{m}}} = e^{-\gamma^{-1} J_D(iy,\gamma)} \; , \quad (2)$$

where $\gamma = \rho/N$ and $J_D(\alpha, \gamma) = \gamma \sum_{\boldsymbol{m}\neq 0} \ln[1 - e^{-\epsilon_{\boldsymbol{m}} - \alpha}]$. The contribution from the $\boldsymbol{m} = 0$ sector can be written in terms of coherent states $|z\rangle$ satisfying $b_0|z\rangle = z|z\rangle$ as follows,

$$\begin{aligned} {\rm Tr}_{\boldsymbol{m}=0} e^{-(\epsilon_0 + iy) b_0^\dagger b_0} &= \int \frac{d^2 z}{\pi} e^{-|z|^2} \langle z | e^{-(\epsilon_0+iy) b_0^\dagger b_0} | z \rangle \\ &= \int \frac{d^2 z}{\pi} \sum_{n=0}^{\infty} \frac{|z|^{2n}}{n!} e^{-|z|^2} e^{-(\epsilon_0 + iy)n} \; , \end{aligned} \quad (3)$$

where $d^2 z = d{\rm Re}z d{\rm Im}z$, and in the second line we have evaluated the matrix element by inserting the resolution of unity in the basis $|n\rangle$ of particle number eigenstates, $b_0^\dagger b_0 |n\rangle = n|n\rangle$. With $\phi = z/\sqrt{N}$ we finally obtain

$$Z_N = \int d^2\phi \, e^{-N\mathcal{L}_N^{\rm SSB}(\phi)} \; , \quad (4)$$

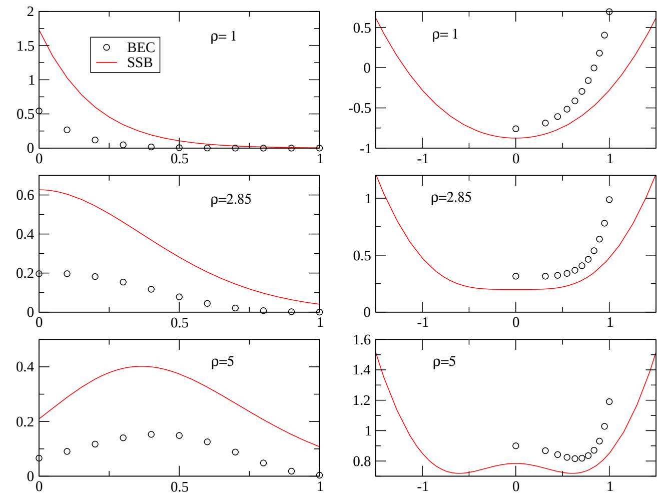

FIG. 2: (Color online) Order parameter probability distributions (left column) and Landau functions (right column) of $N = 10$ bosons in a three-dimensional harmonic potential for different dimensionless densities $\rho = (\lambda_{\rm th}/L)^3 N$. The plots in the second row correspond to the critical density $\rho_c \approx 2.85$ for $N = 10$. Discrete points denote $P_N^{\rm BEC}$ (plotted versus $q = n/N$) and $\mathcal{L}_N^{\rm BEC}$ (versus $\sqrt{q}$), while the continuous curves represent $P_N^{\rm SSB}$ (versus $|\phi|^2$) and $\mathcal{L}_N^{\rm SSB}$ (versus Reϕ).

where the Landau function for SSB is

$$\mathcal{L}_N^{\rm SSB}(\phi) = |\phi|^2 - \frac{1}{N} \ln\Big[\frac{N}{\pi} \sum_{n=0}^{N} \frac{(N|\phi|^2)^n}{n!} e^{-N\mathcal{L}_N^{\rm BEC}(n/N)}\Big] , \quad (5)$$

and the corresponding Landau function for BEC is

$$\mathcal{L}_N^{\rm BEC}(q) = \epsilon_0 q - \frac{1}{N} \ln\Big[\int_0^{2\pi} \frac{dy}{2\pi} e^{iyN(1-q) - \frac{N}{\rho} J_D(iy, \frac{\rho}{N})}\Big] \; . \quad (6)$$

We have normalized the Landau functions such that they are dimensionless and have finite limits for $N \to \infty$. We conclude that the normalized probability density of the order parameter ϕ for SSB is

$$P_N^{\rm SSB}(\phi) = Z_N^{-1} e^{-N\mathcal{L}_N^{\rm SSB}(\phi)} \; , \quad (7)$$

while the probability of observing a fraction $q = n/N$ of bosons in the single-particle state with lowest energy is

$$P_N^{\rm BEC}(q) \;=\; Z_N^{-1} e^{-N\mathcal{L}_N^{\rm BEC}(q)} \; . \quad (8)$$

For HB the probability $P_N^{\rm BEC}(q)$ has been calculated numerically for $N \leq 500$ by Balazs and Bergeman [7] using an efficient recursive algorithm; however, they neither considered the corresponding Landau function nor the analogous quantities for SSB.

In Fig. 2 we show numerical results for the above Landau functions and the associated probability distributions for HB in $D = 3$. Obviously, the behavior is typical for second order phase transitions. We shall show shortly that for HB in $D = 3$ this remains true for $N \to \infty$. In

this limit the critical (dimensionless) density for BEC and SSB in D dimensions is $\rho_c = \zeta(d)$, where $d = D/2$ for FB and $d = D$ for HB. For finite clusters with $N \geq 2$ particles we define the critical density $\rho_c^{\rm BEC}(N)$ for BEC as the value of ρ where $\mathcal{L}_N^{\rm BEC}(0) = \mathcal{L}_N^{\rm BEC}(1/N)$. Analogously, at $\rho = \rho_c^{\rm SSB}(N)$ the minimum of $\mathcal{L}_N^{\rm SSB}(\phi)$ shifts from $\phi = 0$ to $|\phi| > 0$. This definition of the critical density (and the associated critical temperature) in finite clusters is free of ambiguities and remains valid for interacting bosons [5, 6, 9, 10]. Of course, in finite systems one may use other criteria, such as the behavior of the specific heat [14], to define a characteristic temperature which approaches the critical temperature for $N \to \infty$. Numerically we find that even for small clusters containing a few bosons $\rho_c^{\rm BEC}(N) \approx \rho_c^{\rm SSB}(N)$. The most efficient way to obtain the Landau functions is to directly calculate $P_N^{\rm BEC}(q)$ recursively [7], and then use Eqs. (5,7,8). As expected, with increasing N the critical density slowly approaches the bulk value $\rho_c = \zeta(3) \approx 1.09$ from above (for example $\rho_c(100) \approx 1.93$ and $\rho_c(500) \approx 1.60$), and the probability distributions develop narrows peaks, so that the difference between the most probable and the average value of the order parameter vanishes. The advantage of parameterizing the probability distributions in terms of Landau functions is that only their detailed shape (but not their overall scale) depends on N, because the leading N-dependence has already been taken into account via the prefactor N in the exponent $\exp[-N\mathcal{L}_N]$.

In the rest of this work we consider the limit $N \to \infty$ with fixed ρ. For FB this is the usual thermodynamic limit, while for HB this limiting procedure amounts to letting $\omega \to 0$ at fixed $\omega^D N \propto \rho$, see Ref. [2]. Then the summation in Eq. (5) is sharply peaked at $n = N|\phi|^2$, so that $\mathcal{L}_\infty^{\rm SSB}(\phi) = \mathcal{L}_\infty^{\rm BEC}(|\phi|^2) \equiv \mathcal{L}_\infty(|\phi|^2)$ where $\mathcal{L}_\infty(q) = -\lim_{N\to\infty} N^{-1} \ln I_N(q)$, and $I_N(q)$ is the following integral in the complex $z = x + iy$ plane,

$$I_N(q) = \int_0^{2\pi i} \frac{dz}{2\pi i} e^{Nf(z)} \,. \tag{9}$$

The complex function $f(z)$ is in D dimensions given by

$$f(z) = z(1-q) + \rho^{-1} g_{d+1}(z) \,. \tag{10}$$

Recall that $d = D/2$ for FB and $d = D$ for HB. The Bose-Einstein integral $g_s(z)$ is defined by [15]

$$g_s(z) = \frac{1}{\Gamma(s)} \int_0^\infty du \frac{u^{s-1}}{e^{u+z} - 1} \,, \tag{11}$$

were $\Gamma(s)$ is the Γ-function. In the complex z-plane $g_s(z)$ has infinitely many branch points at integer multiples of $2\pi i$, with branch cuts parallel to the negative real axis.

The leading asymptotic behavior of the $I_N(q)$ for large N can be obtained using the method of steepest descends [16]. For $\rho < \rho_c = g_d(0) = \zeta(d)$, or if $\rho > \rho_c$ but $q > q_c = 1 - \rho_c/\rho > 0$, the saddle point equation

$$df(z)/dz = 1 - q - \rho^{-1} g_d(z) = 0 \tag{12}$$

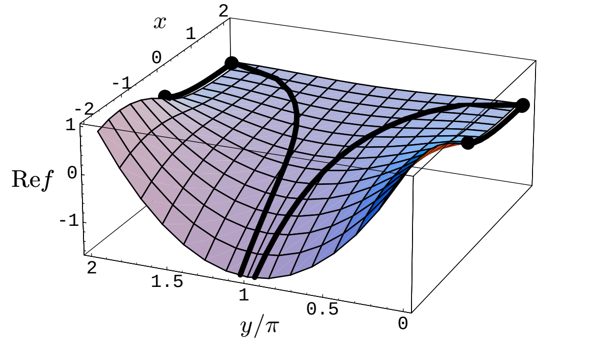

FIG. 3: (Color online) Typical behavior of Re$f(x+iy)$ defined in Eq. (10) in the regime $q > q_c$. The graph is for $d = 3/2$, $q = 0.95$, and $q_c = 0.05$. The end points of the integration and the saddle points are marked by black dots. The thick line marks the value of Ref on a deformation of the original integration contour in Eq. (9) along steepest descend paths through the saddle points $z_0 = \alpha(q,\rho)$ and $z_1 = \alpha(q,\rho) + 2\pi i$.

has a solution $z_0 = \alpha(q,\rho)$ on the positive real axis. Using the analyticity of the integrand, we may then deform the original integration contour into a combination of steepest descend paths through z_0 and the related saddle point $z_1 = \alpha(q,\rho) + 2\pi i$, as shown in Fig. 3. The asymptotic behavior of $I_N(q)$ for $N \to \infty$ is determined by the value of the integrand at the saddle points z_0 and z_1, which yield complex conjugate contributions. We thus obtain in this regime $\mathcal{L}_\infty(q) = -f(\alpha(q,\rho))$. The corresponding effective potential $U_{\rm eff}(\phi) = \mathcal{L}_\infty(|\phi|^2) - \mathcal{L}_\infty(0)$ shows rather non-trivial behavior, in spite of the fact that we are dealing with a non-interacting system. For simplicity, we consider here only the regime close to the phase transition, where $|\rho - \rho_c| \ll \rho_c$. In the normal phase $\rho < \rho_c$ we may expand $U_{\rm eff}$ in powers of $|\phi|^2$,

$$U_{\rm eff}(\phi) = \alpha_0 |\phi|^2 + \frac{u_0}{2}|\phi|^4 + O(|\phi|^6) \,. \tag{13}$$

Here $\alpha_0 = \alpha(q = 0, \rho)$ is the real solution of Eq. (12) for $q = 0$, i.e. $\rho = g_d(\alpha_0)$, and $u_0 = \chi^{-1}(\alpha_0)$, where $\chi(\alpha) = \rho^{-1} g_{d-1}(\alpha)$ is the susceptibility of the Bose gas.

Eq. (13) is the usual behavior of the effective potential in the vicinity of continuous phase transitions. For $\rho \to \rho_c$ the parameter α_0 vanishes, so that at the first sight it seems that the leading term of the effective potential at the critical point is proportional to $|\phi|^4$. However, this conventional scenario is only correct for $d > 2$, i.e. for dimensions $D > 4$ (FB) or $D > 2$ (HB). For $d \leq 2$ the susceptibility $\chi(\alpha)$ diverges for $\alpha \to 0$, implying $u_0 \to 0$ for $\rho \to \rho_c$. For $1 < d < 2$ we find at the critical point to leading order $U_{\rm eff}(\phi) \approx A(\rho_c)|\phi|^{\frac{2d}{d-1}}$ with $A(\rho) = (1 - d^{-1})|\rho/\Gamma(1-d)|^{\frac{1}{d-1}}$. In particular, for FB in $D = 3$ we obtain $U_{\rm eff}(\phi) = \frac{[\zeta(3/2)]^2}{12\pi}|\phi|^6$. In the condensed phase $\rho > \rho_c$ the Landau function for $q > q_c$ is still determined by the above saddle points z_0 and z_1. In this case we obtain close to the phase transition

$$U_{\rm eff}(\phi) \approx \begin{cases} \frac{u_0}{2}(|\phi|^2 - q_c)^2 & \text{for } d > 2 \\ A(\rho)(|\phi|^2 - q_c)^{\frac{d}{d-1}} & \text{for } 2 > d > 1 \end{cases} \,. \tag{14}$$

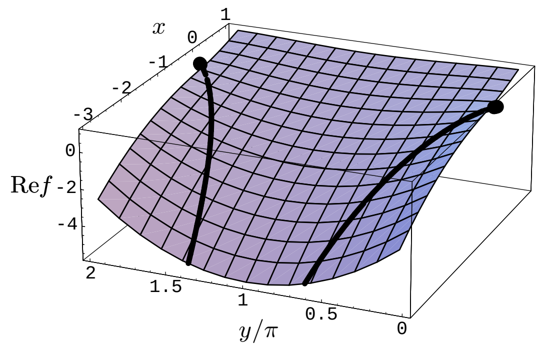

FIG. 4: (Color online) Re$f(x+iy)$ and steepest descend paths for $q < q_c$. The graph is for $d = 3/2$, $q_c = 0.05$, and $q = 0.045$.

Note that for $q > q_c$ the Landau function can be identified with the Gibbs potential for $N \to \infty$, so that the above results can also be derived from thermodynamics.

On the other hand, in the condensed phase $\rho > \rho_c$ the Gibbs potential is constant for $q < q_c = 1 - \rho_c/\rho$, and is not necessarily equal to the Landau function [1]. It turns out that in this regime the saddle point equation (12) does not have solutions on the principal sheet of the Riemann surface of the complex function $f(z)$ defined in Eq. (10). However, there are saddle points on higher sheets, two of which (which we call $\tilde{z}_0$ and $\tilde{z}_1$) are the analytic continuation of the saddle points z_0 and z_1 discussed above for $q > q_c$. While we have not attempted a global analysis of the descend paths on the higher sheets of the Riemann surface of $f(z)$ for arbitrary d, we can show that for $d > 5/3$ the path connecting the origin to $\tilde{z}_0$ continues to be a steepest descend path, so that the saddle points $\tilde{z}_0$ and $\tilde{z}_1$ are still relevant for the asymptotics of $I_N(q)$ for $N \to \infty$. The leading behavior of $\mathcal{L}_\infty(q)$ for small $q_c - q > 0$ can then be obtained by analytic continuation of the corresponding result for $q > q_c$, which amounts to replacing $|\phi|^2 - q_c$ by $q_c - |\phi|^2$ in Eq. (14). Hence, for $d > 5/3$ the effective potential qualitatively resembles the "Mexican hat" characteristic for continuous phase transitions, although for $5/3 < d < 2$ its shape cannot be approximated by a quartic potential [17].

On the other hand, for $1 < d < 5/3$ the saddle points $\tilde{z}_0$ and $\tilde{z}_1$ become *inadmissible* for the asymptotic expansion of $I_N(q)$ in the sense defined on p. 267 of Ref. [16]; the end-points of the integration can then be directly connected by steepest descend paths avoiding any saddle point. For $d = 3/2$ the proper deformation of the integration contour is shown in Fig. 4. As a consequence, for $d < 5/3$ the Landau function is constant $\mathcal{L}_\infty(q) = -\rho^{-1} g_{d+1}(0)$ for $0 < q < q_c = 1 - \rho_c/\rho$, just like the Gibbs potential. Note that in $D = 3$ the behavior of $\mathcal{L}_\infty(q)$ depends on the form of the external potential: while for FB ($d = D/2 = 3/2$) the Landau function has a plateau for $0 < q < q_c$, for HB ($d = D = 3$) it has the "Mexican hat" form.

In summary, we have defined and evaluated the Landau functions and the order parameter probability distributions for BEC and SSB of non-interacting bosons in a canonical ensemble. The shape of the Landau functions in the condensed phase depends on the dimensionality and on the shape of an external potential in a surprisingly complex way. For bosons in a harmonic trap the evolution of the Landau functions with density or temperature is typical for second order phase transitions. The shape of Landau functions leads to the most natural extension of the concept of the critical temperature for BEC and SSB in finite systems.

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